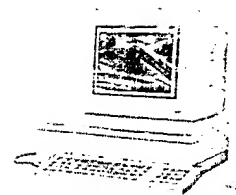


# BioTech-Chem Library

## Search Results

### Feedback Form (Optional)



Scientific & Technical Information Center

The search results generated for your recent request are attached. If you have any questions or comments (compliments or complaints) about the scope or the results of the search, please contact *the BioTech-Chem searcher* who conducted the search *or contact*:

Mary Hale, Supervisor, 308-4258  
CM-1 Room 1E01

---

#### *Voluntary Results Feedback Form*

➤ *I am an examiner in Workgroup:* (Example: 1610)

➤ *Relevant prior art **found**, search results used as follows:*

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

*Types of relevant prior art found:*

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature  
(journal articles, conference proceedings, new product announcements etc.)

➤ *Relevant prior art **not found**:*

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Search results were not useful in determining patentability or understanding the invention.

**Other Comments:**

---

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DICTIONARY FILE UPDATES: 12 FEB 2003 HIGHEST RN 489395-53-1

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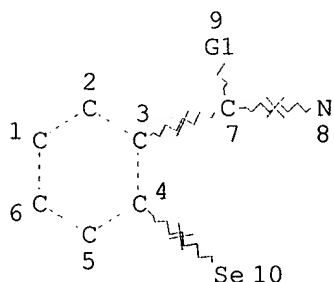
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d sta que 19

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

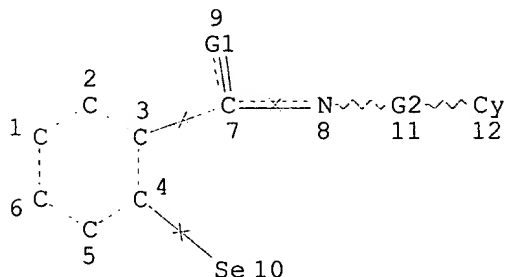
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NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L5 726 SEA FILE=REGISTRY SSS FUL L1

L7 STR



VAR G1=O/S

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REP G2=(0-5) CH2  
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DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE  
L9 461 SEA FILE=REGISTRY SUB=L5 SSS FUL L7

100.0% PROCESSED 726 ITERATIONS  
SEARCH TIME: 00.00.01

461 ANSWERS

=> d his

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SET COST OFF

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L1 STR  
L2 40 S L1  
L3 STR L1  
L4 40 S L3  
L5 726 S L1 FUL  
SAV L5 KUMAR926/A  
L6 STR L1  
L7 STR L6  
L8 17 S L7 SAM SUB=L5  
L9 461 S L7 FUL SUB=L5  
SAV L9 KUMAR926A/A  
L10 STR L7  
L11 4 S L10 SAM SUB=L9  
L12 69 S L10 FUL SUB=L9  
SAV L12 KUMAR926B/A  
L13 STR L10  
L14 197 S L9 AND NSEC3-C6/ES  
L15 2 S L9 AND NSEC3-OCOC2-C6/ES  
L16 262 S L9 NOT L14,L15  
L17 195 S L16 NOT L12  
L18 STR L13  
L19 6 S L9 AND OCOC2-C6/ES  
L20 266 S L12,L14,L15  
L21 195 S L9 NOT L20  
L22 STR L18  
L23 13 S L22 CSS SAM SUB=L9  
L24 254 S L22 CSS FUL SUB=L9  
SAV L24 KUMAR926C/A  
L25 66 S L24 AND L12  
L26 3 S L12 NOT L25  
L27 2 S L26 NOT C28H20N2O6SE2  
L28 254 S L24 AND L16  
L29 8 S L16 NOT L28  
L30 1 S L29 AND C21H17NO3SE  
L31 4 S L19 NOT (C15H13NO3SE OR C14H9NO4SE)  
L32 26 S L28 AND METHYLSELENO  
L33 228 S L28 NOT L32  
L34 85 S L33 AND S/ELS  
L35 15 S L34 AND SULFONYL  
L36 70 S L34 NOT L35

L37 18 S L36 AND GLYCINE  
L38 16 S L37 NOT C18H18N2O4SSE  
L39 52 S L36 NOT L37  
L40 143 S L33 NOT L34-L39

FILE 'HCAPLUS' ENTERED AT 18:49:56 ON 13 FEB 2003

L41 91 S L25,L27,L30,L15,L31,L35,L38,L39,L40  
E HOLMGREN A/AU  
L42 288 S E3-E5,E13  
E AMIRI M/AU  
L43 7 S E3,E8,E10  
E MASAYASU H/AU  
L44 33 S E3,E4  
L45 2 S L41 AND L42-L44  
E DAIICHI/PA,CS  
E DAIICH/PA,CS  
L46 8279 S E3-E18  
E DAICH/PA,CS  
L47 22 S E13,E14  
L48 7 S L41 AND L46,L47  
L49 8 S L45,L48  
L50 8 S L5 AND L49

FILE 'REGISTRY' ENTERED AT 18:54:32 ON 13 FEB 2003

L51 1 S 139015-80-8  
L52 1 S 60940-34-3  
L53 1 S 9074-14-0

FILE 'HCAPLUS' ENTERED AT 18:55:29 ON 13 FEB 2003

L54 696 S L53  
L55 1104 S THIOREDOXIN REDUCTASE OR (NADP OR NADPH) (S)THIOREDOXIN(S)REDU  
L56 1117 S L54,L55  
L57 518 S L5  
L58 7 S L56 AND L57  
L59 112 S L42-L47 AND L56  
L60 3 S L59 AND L57  
L61 14 S L50,L58,L60  
L62 236 S L57 AND ?PEROXID?  
L63 181 S L57 AND (PEROXIDASE OR PEROXIDAT?)  
L64 9 S L61 AND L62,L63  
L65 5 S L61 NOT L64  
SEL DN AN 3 5  
L66 3 S L65 NOT E1-E6  
L67 12 S L64,L66  
SEL HIT RN

FILE 'REGISTRY' ENTERED AT 19:00:36 ON 13 FEB 2003

L68 31 S E7-E37  
L69 14 S L68 AND (C14H13NOSE OR C13H11NO4SE OR C17H15NO5SSE OR C21H27N  
L70 17 S L68 NOT L69  
L71 1 S L69 AND C13H11NO2SE  
L72 16 S L70 NOT C13H11NO3SE  
L73 17 S L71,L72

FILE 'HCAPLUS' ENTERED AT 19:08:46 ON 13 FEB 2003

FILE 'REGISTRY' ENTERED AT 19:09:08 ON 13 FEB 2003

L74 16 S L73 NOT L53

FILE 'HCAPLUS' ENTERED AT 19:09:13 ON 13 FEB 2003

L75 426 S L74  
L76 7 S L75 AND L56  
L77 5 S L67 NOT L76

L78 8 S L45,L76  
L79 1 S L78 NOT L76  
L80 8 S L78,L79

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FILE 'HCAPLUS' ENTERED AT 19:10:56 ON 13 FEB 2003

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FILE LAST UPDATED: 12 Feb 2003 (20030212/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l80 all hitstr tot

L80 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2003 ACS

AN 2002:783160 HCAPLUS

TI A Novel Antioxidant Mechanism of Ebselen Involving Ebselen Diselenide, a Substrate of Mammalian Thioredoxin and **Thioredoxin Reductase**

AU Zhao, Rong; Holmgren, Arne

CS Department of Medical Biochemistry and Biophysics, Medical Nobel Institute for Biochemistry, Karolinska Institutet, Stockholm, SE-171 77; Swed.

SO Journal of Biological Chemistry (2002), 277(42), 39456-39462

CODEN: JBCHA3; ISSN: 0021-9258

PB American Society for Biochemistry and Molecular Biology

DT Journal

LA English

CC 7-3 (Enzymes)

Section cross-reference(s): 6

AB The antioxidant mechanism of ebselen involves recently discovered redns.

by mammalian **thioredoxin reductase** (TrxR) and

thioredoxin (Trx) forming ebselen selenol. Here we describe a previously unknown reaction; ebselen reacts with its selenol forming an ebselen diselenide with a rate const. of 372 M<sup>-1</sup>s<sup>-1</sup>. The diselenide also was a substrate of TrxR forming the selenol with K<sub>m</sub> of 40 .mu.M and k<sub>cat</sub> of 79 min<sup>-1</sup> (k<sub>cat</sub>/K<sub>m</sub> of 3.3 .times. 104 M<sup>-1</sup>s<sup>-1</sup>). Trx increased the redn.

because of its fast reaction with diselenide (rate const. 1.7 .times. 103 M<sup>-1</sup>s<sup>-1</sup>). Diselenide stimulated the H2O2 reductase activity of TrxR, even more efficiently with Trx present. Because the mechanism of ebselen as an antioxidant has been assumed to involve glutathione peroxidase-like activity, we compared the H2O2 reductase activity of ebselen with the GSH and Trx systems. TrxR at 50 nM, far below the estd. physiol. level, gave 8-fold higher activity compared with 1 mM GSH; addn. of 5 .mu.M Trx increased this difference to 13-fold. The rate const. of ebselen selenol reacting with H2O2 was estd. to be faster than 350 M<sup>-1</sup>s<sup>-1</sup>. We propose

novel mechanisms for ebselen antioxidant action involving ebselen selenol and diselenide formation, with the thioredoxin system rather than glutathione as the predominant effector and target.

ST ebselen antioxidant diselenide thioredoxin peroxide reductase

IT INDEXING IN PROGRESS

IT Antioxidants

Enzyme kinetics

Michaelis constant

(novel ebselen antioxidant action involves ebselen selenol and diselenide formation with thioredoxin system as predominant effector and target)

IT Thioredoxins

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(novel ebselen antioxidant action involves ebselen selenol and diselenide formation with thioredoxin system as predominant effector and target)

IT 9074-14-0, Thioredoxin reductase

60940-34-3, Ebselen

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(novel ebselen antioxidant action involves ebselen selenol and diselenide formation with thioredoxin system as predominant effector and target)

RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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IT INDEXING IN PROGRESS

IT 9074-14-0, **Thioredoxin reductase**

60940-34-3, Ebselen

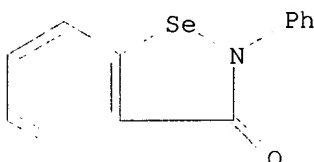
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(novel ebselen antioxidant action involves ebselen selenol and  
diselenide formation with thioredoxin system as predominant effector  
and target)

RN 9074-14-0 HCAPLUS

CN Reductase, thioredoxin (9CI) (CA INDEX NAME)

RN 60940-34-3 HCAPLUS

CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



L80 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2003 ACS

AN 2002:519211 HCAPLUS

DN 138:83310

TI Ebselen: a substrate for human **thioredoxin reductase**  
strongly stimulating its hydroperoxide reductase activity and a superfast  
thioredoxin oxidant

AU Zhao, Rong; Masayasu, Hiroyuki; Holmgren, Arne

CS Medical Nobel Institute for Biochemistry, Department of Medical  
Biochemistry and Biophysics, Karolinska Institute, Stockholm, SE-171 77,  
Swed.

SO Proceedings of the National Academy of Sciences of the United States of  
America (2002), 99(13), 8579-8584

CODEN: PNASA6; ISSN: 0027-8424

PB National Academy of Sciences

DT Journal

LA English

CC 1-12 (Pharmacology)

AB Ebselen [2-phenyl-1,2-benzisoselenazol-3(2H)-one], a seleno-org. compd.  
with glutathione peroxidase-like activity is used in clin. trials against  
stroke. Human and bovine TrxR catalyzed the redn. of ebselen to ebselen  
selenol by NADPH with an apparent KM-value of 2.5 .mu.M and a kcat of 588  
min-1. The addn. of thioredoxin (Trx) stimulated the TrxR-catalyzed redn.  
of ebselen several-fold. This result was caused by a very fast oxidn. of  
reduced Trx by ebselen with a rate const. in excess of 2.times.107 M-1  
s-1. This rate is orders of magnitude faster than the reaction of dithiol

Trx with insulin disulfides. Ebselen competed with disulfide substrates for redn. by Trx and, therefore, acted as an inhibitor of protein disulfide redn. by the Trx system. The inherent H<sub>2</sub>O<sub>2</sub> reductase activity of mammalian TrxR dependent on its active-site selenocysteine residue was stimulated 10-fold by 2 .mu.M ebselen and 25-fold in the addnl. presence of 5 .mu.M Trx. Furthermore, the apparent KM-value of TrxR for H<sub>2</sub>O<sub>2</sub> was lowered 25-fold to about 100 .mu.M. Our results demonstrate that ebselen is a TrxR peroxidase which, in the presence of Trx, acted as a mimic of a peroxiredoxin. The activity with TrxR and oxidn. of reduced Trx offer mechanistic explanations for the in vivo effects of ebselen as an antioxidant and anti-inflammatory agent. Our results demonstrate that the mechanism of action of ebselen may be predominantly via the Trx system rather than via glutathione.

ST ebselen **thioredoxin reductase** hydroperoxide  
antioxidant human **NADPH**

IT Anti-inflammatory agents  
Antioxidants  
Human

(ebselen is a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide reductase activity and a superfast thioredoxin oxidant)

IT Brain, disease  
(stroke; ebselen is a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide reductase activity and a superfast thioredoxin oxidant)

IT 53-57-6, **NADPH** 9013-66-5, Glutathione peroxidase  
**9074-14-0, Thioredoxin reductase**  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(ebselen is a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide reductase activity and a superfast **thioredoxin** oxidant)

IT **60940-34-3, Ebselen**  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(ebselen is a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide reductase activity and a superfast thioredoxin oxidant)

RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE

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IT 9074-14-0, **Thioredoxin reductase**

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (ebselen is a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide reductase activity and a superfast thioredoxin oxidant)

RN 9074-14-0 HCAPLUS

CN Reductase, thioredoxin (9CI) (CA INDEX NAME)

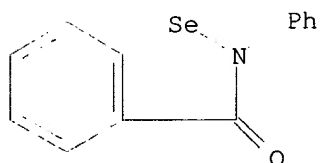
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IT 60940-34-3, Ebselen

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (ebselen is a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide reductase activity and a superfast thioredoxin oxidant)

RN 60940-34-3 HCAPLUS

CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



L80 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2003 ACS

AN 2001:669761 HCAPLUS

DN 136:35047

TI The biochemistry of selenium and the glutathione system

AU Arteel, G. E.; Sies, H.

CS Department of Pharmacology, Laboratory of Hepatobiology and Toxicology, University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599-7365, USA

SO Environmental Toxicology and Pharmacology (2001), 10(4), 153-158

CODEN: ETOPFR; ISSN: 1382-6689

PB Elsevier Science B.V.

DT Journal; General Review

LA English

CC 13-0 (Mammalian Biochemistry)

Section cross-reference(s): 1

AB A review. In the context of defense against pro-oxidants, selenium and the glutathione (GSH) system play key functions. Major roles of GSH include direct interception of pro-oxidants, as well as a redn. of other

antioxidants from their oxidized forms. Furthermore, GSH has ancillary functions, such as metab., cell signaling, and protein interactions, that can also mediate defense against oxidants. Protection by selenium in the mammalian cell is mediated by selenol-amino acids, either as selenocystine or selenomethionine. The active site of the potent glutathione peroxidases (GPx) contains selenocystine residues. Furthermore, other selenoproteins (e.g. selenoprotein P and **thioredoxin reductase**) also have been shown to possess antioxidant properties. Synthetic organoselenium compds. (e.g. ebselen) have also shown promise as pharmacol. antioxidants in in vivo models of tissue damage due to oxidative stress. The specific function of selenoproteins and organoselenium compds. in defense against peroxynitrite, by redn. of this potent oxidizing and nitrating species to nitrite, is also discussed.

- ST review selenium glutathione peroxynitrite oxidative stress antioxidant; ebselen antioxidant glutathione peroxidase selenoprotein oxidative stress review
- IT Antioxidants  
(biochem. of selenium and glutathione system)
- IT Antioxidants  
Oxidative stress, biological  
(biochem. of selenium and glutathione system in relation to)
- IT Proteins  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(selenium-contg.; biochem. of selenium and glutathione system)
- IT 70-18-8, Glutathione, biological studies 7782-49-2, Selenium, biological studies 9013-66-5, Glutathione peroxidase  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(biochem. of selenium and glutathione system)
- IT 19059-14-4, Peroxynitrite  
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)  
(biochem. of selenium and glutathione system in relation to)
- IT **60940-34-3**, Ebselen  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(biochem. of selenium and glutathione system in relation to)

RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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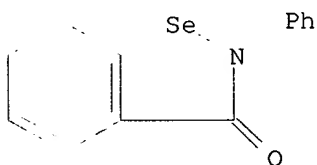
IT 60940-34-3, Ebselen

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
(Biological study); USES (Uses)

(biochem. of selenium and glutathione system in relation to)

RN 60940-34-3 HCAPLUS

CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



L80 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2003 ACS

AN 2000:707140 HCAPLUS

DN 133:271642

TI Use of 2-phenyl-1,2-benzisoselenazol-3(2H)-one or its derivatives as  
substrates for thioredoxin reductase

IN Holmgren, Arne; Amiri, Marjan H.; Masayasu,

**Hiroyuki**

PA Daiichi Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

IC ICM C07C391-02

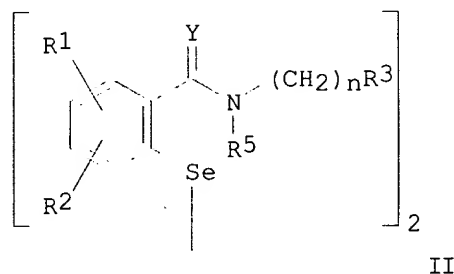
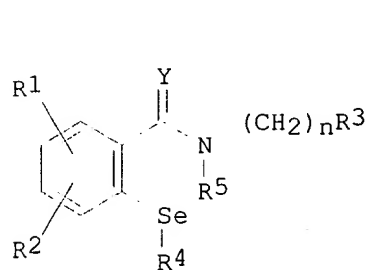
ICS A61K031-166; A61P039-06; B01J031-12; C07B031-00; C09K015-32;  
C12N009-00; C12N009-04

CC 63-5 (Pharmaceuticals)

Section cross-reference(s): 1, 7

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000058281	A1	20001005	WO 2000-JP2076	20000331
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	EP 1174423	A1	20020123	EP 2000-913022	20000331
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
PRAI	JP 1999-92789	A	19990331		
	JP 1999-101478	A	19990408		
	WO 2000-JP2076	W	20000331		
OS	MARPAT 133:271642				
GI					



AB Substrates for **thioredoxin reductase**, contg. compds. represented by general formula (I) or (II) (such as 2-phenyl-1,2-benzisoselenazol-3(2H)-one (III) or open-ring derivs. thereof) (wherein R1 and R2 are each hydrogen, halogeno, trifluoromethyl, NO2, C1-6 alkyl or alkoxy; or R1 and R3 are combined together represent methylenedioxy; R3 is (un)substituted aryl, arom. heterocyclic group, or 5- to 7-membered cycloalkyl or cycloalkenyl; R4 is hydrogen, hydroxyl, an -S-.alpha.-amino acid group, or aralkyl optionally having 1 or .gtoreq.2 substituents; R5 is hydrogen or C1-6 alkyl; Y is oxygen or sulfur; and n is an integer of 0 to 5, with the proviso that the selenium atom may be oxidized) are described. These substrates are reduced by **thioredoxin reductase** in the presence of **NADPH** and enhance the peroxidase activity of **thioredoxin reductase**. A tablet formulation contg. III 50, CM-cellulose 25, starch 5, cryst. cellulose 40, and magnesium stearate 2 mg was prepd.

ST phenylbenzisoselenazolone substrate **thioredoxin**

**reductase; peroxidase activity enhancement thioredoxin reductase**

IT 139015-80-8

RL: ANT (Analyte); BSU (Biological study, unclassified); MFM (Metabolic formation); PEP (Physical, engineering or chemical process); ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)

(substrates for **thioredoxin reductase**)

IT 60940-34-3, 2-Phenyl-1,2-benzisoselenazol-3(2H)-one

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(substrates for **thioredoxin reductase**)

IT 9074-14-0, **Thioredoxin reductase**

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)

(substrates for **thioredoxin reductase**)

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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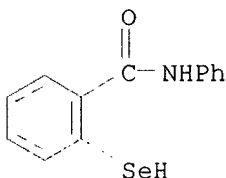
IT 139015-80-8

RL: ANT (Analyte); BSU (Biological study, unclassified); MFM (Metabolic formation); PEP (Physical, engineering or chemical process); ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)

(substrates for **thioredoxin reductase**)

RN 139015-80-8 HCAPLUS

CN Benzamide, N-phenyl-2-selenyl- (9CI) (CA INDEX NAME)



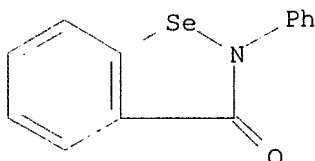
IT 60940-34-3, 2-Phenyl-1,2-benzisoselenazol-3(2H)-one

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(substrates for **thioredoxin reductase**)

RN 60940-34-3 HCAPLUS

CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



IT 9074-14-0, **Thioredoxin reductase**

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
(substrates for **thioredoxin reductase**)

RN 9074-14-0 HCAPLUS

CN Reductase, thioredoxin (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

L80 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2003 ACS

AN 2000:531379 HCAPLUS

DN 133:306449

TI Interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics

AU Sies, H.; Arteel, G. E.

CS Institut fur Physiologische Chemie I, Heinrich-Heine-Universitat Dusseldorf, Dusseldorf, Germany

SO Free Radical Biology & Medicine (2000), 28(10), 1451-1455

CODEN: FRBMEH; ISSN: 0891-5849

PB Elsevier Science Inc.

DT Journal

LA English

CC 4-3 (Toxicology)

Section cross-reference(s): 10

AB Peroxynitrite is an oxidant generated under inflammatory conditions, acting in defense against invading microorganisms. There is a need for protection of the organism from damage inflicted by peroxynitrite. Selenium-contg. compds., notably Ebselen, have a high second-order reaction rate const. (.apprx.2 .times. 10<sup>6</sup> M<sup>-1</sup> s<sup>-1</sup>), which makes them candidates for efficient protection. This applies also for selenium in proteins, occurring as selenocysteine or selenomethionine residues. Glutathione peroxidases, **thioredoxin reductase**, and selenoprotein P have been shown to play a potential role in protection against peroxynitrite. Tellurium-contg. compds. also react with peroxynitrite.

ST peroxynitrite interaction selenoprotein glutathione peroxidase

IT Oxidative stress, biological

(interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)

IT Radicals, biological studies

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

(interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)

IT Proteins, specific or class

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

(selenium-contg., P; interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)

IT Proteins, specific or class

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

(selenium-contg.; interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)

IT 19059-14-4, Peroxynitrite

RL: ADV (Adverse effect, including toxicity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

(interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)

IT 1464-42-2, Selenomethionine 3614-08-2, Selenocysteine 9013-66-5, Glutathione peroxidase 9074-14-0, **Thioredoxin**

**reductase** 13494-80-9D, Tellurium, org. compds., biological studies **60940-34-3**, Ebselen

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

(interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)

RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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IT **9074-14-0, Thioredoxin reductase**  
**60940-34-3**, Ebselen

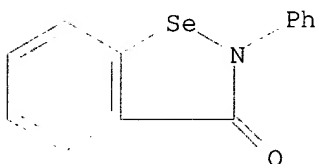
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

(interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)

RN 9074-14-0 HCAPLUS  
 CN Reductase, thioredoxin (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 60940-34-3 HCAPLUS  
 CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



L80 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2003 ACS

AN 1999:117100 HCAPLUS

DN 130:308314

TI Function of **Thioredoxin Reductase** as a Peroxynitrite Reductase Using Selenocystine or Ebselen

AU Arteel, Gavin E.; Briviba, Karlis; Sies, Helmut

CS Institut fuer Physiologische Chemie I, Heinrich-Heine-Universitaet Duesseldorf, Duesseldorf, D-40001, Germany

SO Chemical Research in Toxicology (1999), 12(3), 264-269  
 CODEN: CRTOEC; ISSN: 0893-228X

PB American Chemical Society

DT Journal

LA English

CC 7-3 (Enzymes)

Section cross-reference(s): 4

AB The activity of mammalian **thioredoxin reductase** as a peroxynitrite reductase was investigated. Peroxynitrite was infused to maintain a 0.2 .mu.M steady-state concn. in potassium phosphate buffer (pH 7.4). Benzoate hydroxylation and nitrite formation were used as indexes of oxidn. reactions of peroxynitrite and of peroxynitrite redn., resp. In the presence of **NADPH** (10 .mu.M), **thioredoxin reductase** at 50 nM alone did not significantly scavenge peroxynitrite, as shown by there being no significant effect on benzoate hydroxylation or nitrite formation. However, when selenocystine (1 .mu.M) or ebselen (2 .mu.M) was present in the reaction mixt., there was significant suppression of benzoate hydroxylation and an increase in nitrite formation until all the **NADPH** was oxidized. The addn. of thioredoxin did not enhance these effects. In contrast, peroxynitrite redn. by ebselen complexed with BSA was enhanced by the presence of thioredoxin. In parallel expts., **thioredoxin reductase** efficiently reduced ebselen selenoxide back to ebselen.

ST **thioredoxin reductase** peroxynitrite redn selenocystine ebselen

IT Thioredoxins

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (function of **thioredoxin reductase** as a peroxynitrite reductase using selenocystine or ebselen)

IT Albumins, biological studies

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
 (serum, ebselen complexes; function of **thioredoxin reductase** as a peroxynitrite reductase using selenocystine or ebselen)

IT 9074-14-0, **Thioredoxin Reductase**

60940-34-3D, Ebselen, complexes with bovine serum albumin



RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(function of **thioredoxin reductase** as a peroxynitrite reductase using selenocystine or ebselen)

IT 53-57-6, **Nadph** 19059-14-4, Peroxynitrite 29621-88-3, L-Selenocystine **60940-34-3**, Ebselen 104473-83-8, Ebselen selenoxide

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(function of **thioredoxin reductase** as a peroxynitrite **reductase** using selenocystine or ebselen)

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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IT 9074-14-0, **Thioredoxin Reductase**

**60940-34-3D**, Ebselen, complexes with bovine serum albumin

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(function of **thioredoxin reductase** as a peroxynitrite reductase using selenocystine or ebselen)

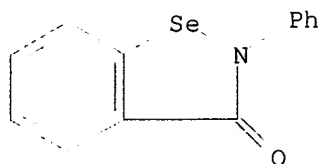
RN 9074-14-0 HCAPLUS

CN Reductase, thioredoxin (9CI) (CA INDEX NAME)

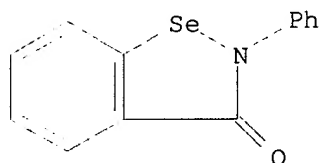
\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 60940-34-3 HCAPLUS

CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



IT 60940-34-3, Ebselen  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (function of **thioredoxin reductase** as a  
 peroxynitrite **reductase** using selenocystine or ebselen)  
 RN 60940-34-3 HCAPLUS  
 CN 1,2-Benziselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



L80 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2003 ACS  
 AN 1998:200706 HCAPLUS  
 DN 128:265859  
 TI Diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents  
 AU Engman, Lars; Cotgreave, Ian; Angulo, Miguel; Taylor, Charles W.; Paine-Murrieta, Gillian D.; Powis, Garth  
 CS Department of Organic Chemistry, Institute of Chemistry, Uppsala University, Uppsala, 75121, Swed.  
 SO Anticancer Research (1997), 17(6D), 4599-4605  
 CODEN: ANTRD4; ISSN: 0250-7005  
 PB Anticancer Research  
 DT Journal  
 LA English  
 CC 1-6 (Pharmacology)  
 AB **Thioredoxin reductase** is a selenocysteine contg. flavoenzyme that catalyzes the **NADPH** dependent redn. of the redox protein **thioredoxin**. Thioredoxin is over-expressed by a no. of human tumors. Exptl. studies have shown that thioredoxin is responsible for the growth and transformed phenotype of some human cancer cells. Thus, **thioredoxin reductase** presents an attractive target for anticancer drug development to regulate the activity of the thioredoxin system. We have examd. a series of 12 organoselenium compds. and 16 organotellurium compds., mostly of the diaryl chalcogenide type, as inhibitors of human **thioredoxin reductase** and have investigated the cytotoxicity and antitumor activity of some of the compds. The organoselenium compd. Ebselen was found to be a competitive inhibitor of human **thioredoxin reductase** ( $K_i$  2.8  $\mu\text{M}$ ), while a no. of organotellurium compds. were found to be noncompetitive inhibitors ( $K_i$ s 2.3 to 35.2  $\mu\text{M}$ ). Human glutathione reductase was not appreciably inhibited by any of the compds., except for one dinitro organotellurium compd. that caused inhibition with an  $IC_{50}$  of 0.5  $\mu\text{M}$  and an over 20-fold selectivity compared to **thioredoxin reductase**. The compds. inhibited the growth of human cancer cells in culture with  $IC_{50}$ s as low as 2  $\mu\text{M}$ . Some organotellurium compds. when administered daily by i.p. injection to mice caused up to 50% inhibition

of the growth of MCF-7 human breast cancer xenografts but the relative insoly. of the compds. was a limiting factor in their use.

ST diaryl chalcogenide **thioredoxin reductase** antitumor

IT Antitumor agents

(diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

IT 149902-64-7P 205675-82-7P

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

IT 35050-01-2 59130-74-4 **60940-34-3** 63212-74-8 65130-25-8  
67516-66-9 77422-94-7 87345-08-2 96636-40-7 96748-33-3  
104755-32-0 117402-62-7 135085-11-9 144381-99-7 144382-00-3  
144382-01-4 144693-22-1 **144842-35-3** 152943-38-9  
152943-49-2 155228-86-7 155228-87-8 155228-88-9 204519-52-8  
205675-80-5 205675-81-6

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

IT 9001-48-3, Glutathione reductase

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

IT 110-02-1, Thiophene 112-89-0, Octadecyl bromide 77422-85-6  
102945-08-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

IT **9074-14-0, Thioredoxin reductase**

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(inhibitors; diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

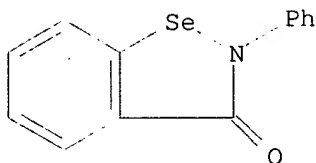
IT **60940-34-3 144842-35-3**

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

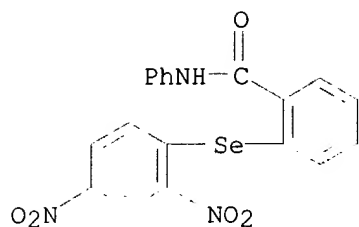
RN 60940-34-3 HCAPLUS

CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



RN 144842-35-3 HCAPLUS

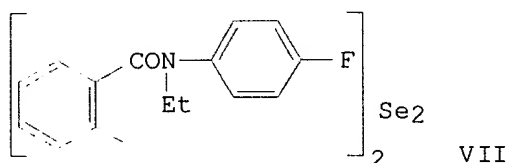
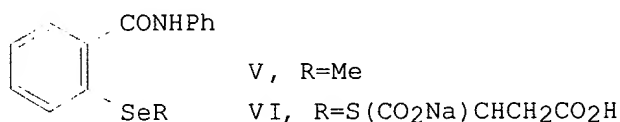
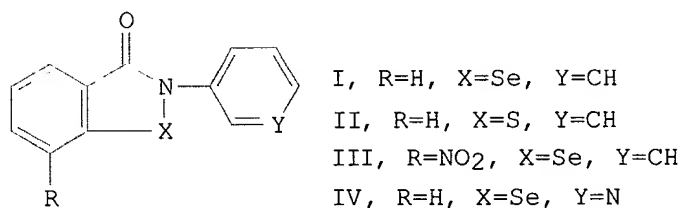
CN Benzamide, 2-[(2,4-dinitrophenyl)seleno]-N-phenyl- (9CI) (CA INDEX NAME)



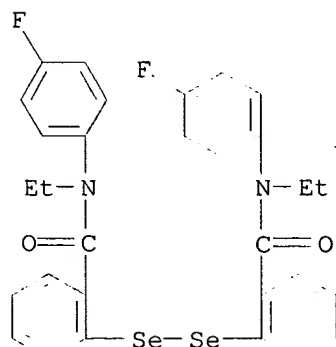
IT 9074-14-0, **Thioredoxin reductase**  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (inhibitors; diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)  
 RN 9074-14-0 HCAPLUS  
 CN Reductase, thioredoxin (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

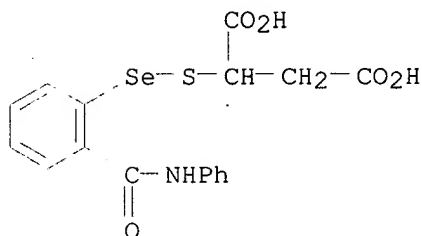
L80 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2003 ACS  
 AN 1990:565101 HCAPLUS  
 DN 113:165101  
 TI Mechanism for the inhibitory effect of a seleno-organic compound, ebselen, and its analogs on superoxide anion production in guinea pig polymorphonuclear leukocytes  
 AU Wakamura, Kyoko; Ohtsuka, Toshiaki; Okamura, Naoki; Ishibashi, Sadahiko; **Masayasu, Hiroyuki**  
 CS Sch. Med., Hiroshima Univ., Hiroshima, 734, Japan  
 SO Journal of Pharmacobio-Dynamics (1990), 13(7), 421-5  
 CODEN: JOPHDQ; ISSN: 0386-846X  
 DT Journal  
 LA English  
 CC 1-7 (Pharmacology)  
 GI



- AB Effects of ebselen (I) and its analogs (PZ-25 (II), NAT06-123 (III), NAT02-761 (IV), NAT02-801 (V), NAT06-099 (VI), and NAT06-513 (VII)) on superoxide anion (O<sub>2</sub><sup>-</sup>) prodn. induced by tetradecanoyl phorbol acetate (TPA) were examd. in intact guinea pig polymorphonuclear leukocytes (PMNL). Four compds. having a structure of 1,2 benzoisoselenazol-3-(2H)one (I, III, IV) and its sulfur-substituted analog (II), had a potent inhibitory effect on O<sub>2</sub><sup>-</sup> prodn. as compared with others. I and III also markedly inhibited NADP (NADPH) oxidase activity, which is responsible for O<sub>2</sub><sup>-</sup> prodn. in intact cells, and in a particulate fraction prepd. from TPA-stimulated PMNL, whereas II inhibited this enzyme weakly and I did not. On the other hand, I and II had the same degree of potent inhibitory effect on protein kinase C which was involved in the regulation of NADPH oxidase activation. Thus, it is plausible that inhibition of O<sub>2</sub><sup>-</sup> prodn. in intact PMNL by these compds. were due not only to direct inhibition of NADPH oxidase but also to inhibition of protein kinase C.
- ST ebselen superoxide formation inhibition polymorphonuclear leukocyte
- IT Inflammation inhibitors  
(ebselen and analogs as)
- IT Leukocyte  
(polymorphonuclear, superoxide formation by, ebselen and analogs inhibition of)
- IT 9026-43-1, Protein kinase  
RL: BIOL (Biological study)  
(C, in polymorphonuclear leukocytes, ebselen and analogs effect on)
- IT 7782-44-7D, Oxygen, radicals 11062-77-4, Superoxide  
RL: FORM (Formation, nonpreparative)  
(formation of, by polymorphonuclear leukocytes, ebselen and analogs inhibition of)
- IT 9032-22-8, NADPH oxidase  
RL: BIOL (Biological study)  
(in polymorphonuclear leukocytes, ebselen and analogs effect on)
- IT 2527-03-9, PZ 25 60940-24-1, NAT 06-099 60940-34-3, Ebselen  
89780-24-5, NAT 06-123 118528-47-5, NAT 02-801 119214-92-5,  
NAT 02-761 129836-90-4, NAT 06-513  
RL: BIOL (Biological study)  
(superoxide formation by polymorphonuclear leukocytes inhibition by)
- IT 7782-49-2D, Selenium, org. compds.  
RL: BIOL (Biological study)  
(superoxide formation by polymorphonuclear leukocytes inhibition by ebselen and analogs as)
- IT 118528-47-5, NAT 02-801 129836-90-4, NAT 06-513  
RL: BIOL (Biological study)  
(superoxide formation by polymorphonuclear leukocytes inhibition by)
- RN 118528-47-5 HCAPLUS
- CN Benzamide, 2,2'-diselenobis[N-ethyl-N-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 129836-90-4 HCAPLUS  
 CN Butanedioic acid, [[[2-[(phenylamino)carbonyl]phenyl]seleno]thio]-,  
 monosodium salt (9CI) (CA INDEX NAME)



● Na

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(FILE 'USPATFULL, USPAT2' ENTERED AT 19:11:44 ON 13 FEB 2003)

L81 35 S L74  
 L82 43 S L9  
 L83 136 S L56  
 L84 0 S L81,L82 AND L83  
 L85 43 S L81,L82  
 L86 35 S L85 AND A61K/IC, ICM, ICS  
 L87 34 S L85 AND (424 OR 514)/NCLM, NCLS  
 L88 8 S L85 NOT L86,L87  
 L89 4 S L88 NOT (SILVER OR GRIP OR DISKS)/TI  
 L90 39 S L86,L87,L89  
 L91 38 S L90 AND (PD<=20000331 OR PRD<=20000331 OR AD<=20000331)

FILE 'REGISTRY' ENTERED AT 19:15:41 ON 13 FEB 2003

FILE 'USPATFULL, USPAT2' ENTERED AT 19:15:41 ON 13 FEB 2003

SET SMARTSELECT ON  
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 SET SMARTSELECT OFF

FILE 'REGISTRY' ENTERED AT 19:15:44 ON 13 FEB 2003

L93 495 S L92  
 L94 0 S L93 AND L74  
 L95 0 S L93 AND L9  
 L96 19 S L93 AND L5  
 L97 2 S L96 AND C22H21NOSE

FILE 'USPATFULL, USPAT2' ENTERED AT 19:17:48 ON 13 FEB 2003

L98 1 S L97

=> fil uspatall

FILE 'USPATFULL' ENTERED AT 19:18:04 ON 13 FEB 2003  
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FILE 'USPAT2' ENTERED AT 19:18:04 ON 13 FEB 2003  
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=> d bib abs hitstr

L98 ANSWER 1 OF 1 USPATFULL

AN 92:70344 USPATFULL

TI Anti-inflammatory benzylselenobenzamides made from anilines and benzylamines

IN Evers, Michel, Liege, Belgium

Fischer, Hartmut, Cologne, Germany, Federal Republic of

Biedermann, Jorgen, Pulheim, Germany, Federal Republic of

Terlinden, Rolf, Cologne, Germany, Federal Republic of

Leyck, Sigurd, Pulheim, Germany, Federal Republic of

PA A. Nattermann &amp; Cie. GmbH, Cologne, Germany, Federal Republic of (non-U.S. corporation)

PI US 5141955 19920825

AI US 1990-611272 19901108 (7)

PRAI DE 1989-3937169 19891108

DT Utility

FS Granted

EXNAM Primary Examiner: Daus, Donald G.

LREP Dubno, Herbert

CLMN Number of Claims: 5

ECL Exemplary Claim: 1

DRWN No Drawings

LN.CNT 621

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Anti-inflammatory benzylselenobenzamides made from anilines and benzylamines have the formula I ##STR1## are disclosed wherein R is hydrogen, methyl or ethyl;

R.sup.1 and R.sup.2 are the same or different and, taken separately, are hydrogen, fluorine, chlorine, bromine, C.sub.1 to C.sub.4 alkyl, C.sub.1 to C.sub.4 alkoxy, hydroxy, cyano, amino, dimethylamino or nitro; and

R.sup.3 and R.sup.4 are the same or different and, taken separately, are hydrogen, fluorine, chlorine, bromine, C.sub.1 to C.sub.4 alkyl, C.sub.1 to C.sub.4 alkoxy, hydroxy, cyano, or nitro and, taken together, represent methylenedioxy; and

n is 0.1 or 2.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

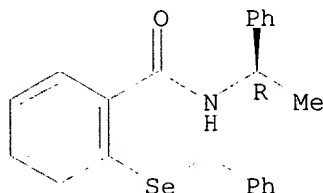
IT 135963-72-3P 135963-73-4P

(prepn. of, as antiinflammatory)

RN 135963-72-3 USPATFULL

CN Benzamide, N-(1-phenylethyl)-2-[(phenylmethyl)seleno]-, (R)- (9CI) (CA INDEX NAME)

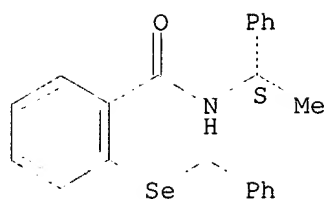
Absolute stereochemistry.



RN 135963-73-4 USPATFULL

CN Benzamide, N-(1-phenylethyl)-2-[(phenylmethyl)seleno]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d his

(FILE 'HOME' ENTERED AT 18:18:58 ON 13 FEB 2003)  
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L4          40 S L3
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L6          STR L1
L7          STR L6
L8          17 S L7 SAM SUB=L5
L9          461 S L7 FUL SUB=L5
           SAV L9 KUMAR926A/A
L10         STR L7
L11         4 S L10 SAM SUB=L9
L12         69 S L10 FUL SUB=L9
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L16         262 S L9 NOT L14,L15
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L18         STR L13
L19         6 S L9 AND OCOC2-C6/ES
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L21         195 S L9 NOT L20
L22         STR L18
L23         13 S L22 CSS SAM SUB=L9
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           SAV L24 KUMAR926C/A
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L27         2 S L26 NOT C28H20N2O6SE2
L28         254 S L24 AND L16
L29         8 S L16 NOT L28
L30         1 S L29 AND C21H17NO3SE
L31         4 S L19 NOT (C15H13NO3SE OR C14H9NO4SE)
L32         26 S L28 AND METHYLSELENO
L33         228 S L28 NOT L32
L34         85 S L33 AND S/ELS
L35         15 S L34 AND SULFONYL
L36         70 S L34 NOT L35
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L42 288 S E3-E5,E13  
E AMIRI M/AU  
L43 7 S E3,E8,E10  
E MASAYASU H/AU  
L44 33 S E3,E4  
L45 2 S L41 AND L42-L44  
E DAIICHI/PA,CS  
E DAIICH/PA,CS  
L46 8279 S E3-E18  
E DAICH/PA,CS  
L47 22 S E13,E14  
L48 7 S L41 AND L46,L47  
L49 8 S L45,L48  
L50 8 S L5 AND L49

FILE 'REGISTRY' ENTERED AT 18:54:32 ON 13 FEB 2003

L51 1 S 139015-80-8  
L52 1 S 60940-34-3  
L53 1 S 9074-14-0

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L54 696 S L53  
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L56 1117 S L54,L55  
L57 518 S L5  
L58 7 S L56 AND L57  
L59 112 S L42-L47 AND L56  
L60 3 S L59 AND L57  
L61 14 S L50,L58,L60  
L62 236 S L57 AND ?PEROXID?  
L63 181 S L57 AND (PEROXIDASE OR PEROXIDAT?)  
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SEL DN AN 3 5  
L66 3 S L65 NOT E1-E6  
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SEL HIT RN

FILE 'REGISTRY' ENTERED AT 19:00:36 ON 13 FEB 2003

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FILE 'REGISTRY' ENTERED AT 19:09:08 ON 13 FEB 2003

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L78 8 S L45,L76  
L79 1 S L78 NOT L76  
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FILE 'REGISTRY' ENTERED AT 19:10:46 ON 13 FEB 2003

FILE 'HCAPLUS' ENTERED AT 19:10:56 ON 13 FEB 2003

FILE 'USPATFULL, USPAT2' ENTERED AT 19:11:44 ON 13 FEB 2003

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L82 43 S L9  
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L85 43 S L81,L82  
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L87 34 S L85 AND (424 OR 514)/NCLM, NCLS  
L88 8 S L85 NOT L86,L87  
L89 4 S L88 NOT (SILVER OR GRIP OR DISKS)/TI  
L90 39 S L86,L87,L89  
L91 38 S L90 AND (PD<=20000331 OR PRD<=20000331 OR AD<=20000331)

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FILE 'REGISTRY' ENTERED AT 19:15:44 ON 13 FEB 2003

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L95 0 S L93 AND L9  
L96 19 S L93 AND L5  
L97 2 S L96 AND C22H21NOSE

FILE 'USPATFULL, USPAT2' ENTERED AT 19:17:48 ON 13 FEB 2003

L98 1 S L97

FILE 'USPATFULL, USPAT2' ENTERED AT 19:18:04 ON 13 FEB 2003

=> fil reg

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DICTIONARY FILE UPDATES: 12 FEB 2003 HIGHEST RN 489395-53-1

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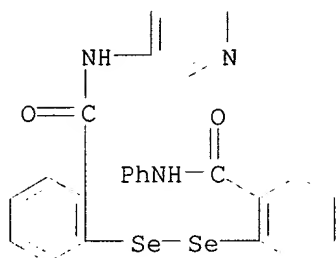
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d scan 125

L25 66 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzamide, 2-[[2-[(phenylamino)carbonyl]phenyl]diseleno]-N-3-pyridinyl-

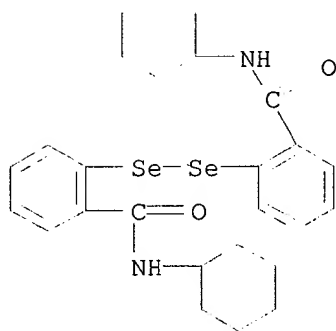
(9CI)  
MF C25 H19 N3 O2 Se2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

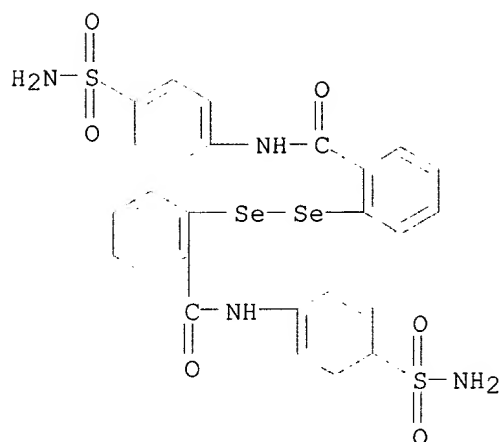
L25 66 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzamide, 2,2'-diselenobis[N-cyclohexyl- (9CI)  
MF C26 H32 N2 O2 Se2



From here to end  
"free" view of  
sample compounds

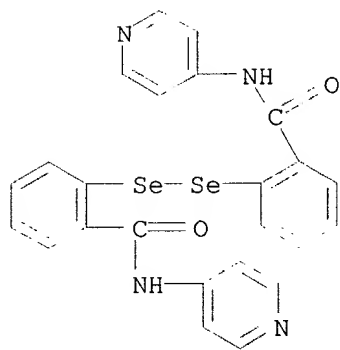
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L25 66 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzamide, 2,2'-diselenobis[N-[4-(aminosulfonyl)phenyl]- (9CI)  
MF C26 H22 N4 O6 S2 Se2



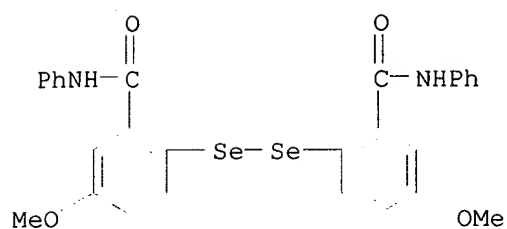
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L25 66 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, 2,2'-diselenobis[N-4-pyridinyl- (9CI)  
 MF C24 H18 N4 O2 Se2



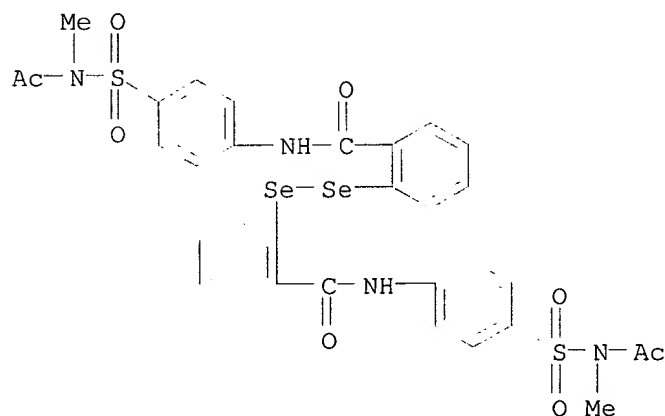
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L25 66 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, 2,2'-diselenobis[5-methoxy-N-phenyl- (9CI)  
 MF C28 H24 N2 O4 Se2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L25 66 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, 2,2'-diselenobis[N-[4-[(acetylmethylamino)sulfonyl]phenyl]-  
 (9CI)  
 MF C32 H30 N4 O8 S2 Se2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

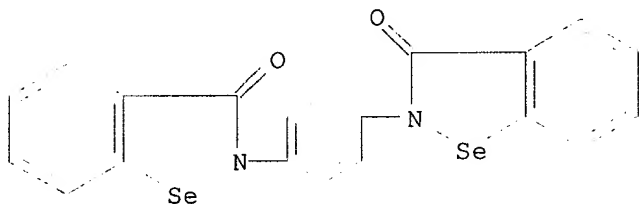
=> d sca 127

L27 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 1,2-Benzisoselenazol-3(2H)-one, 2,2'-[1,1'-biphenyl]-4,4'-diylbis- (9CI)  
 MF C26 H16 N2 O2 Se2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

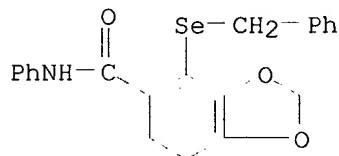
L27 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 1,2-Benzisoselenazol-3(2H)-one, 2,2'-(1,4-phenylene)bis- (9CI)  
 MF C20 H12 N2 O2 Se2



ALL ANSWERS HAVE BEEN SCANNED

=> d sca 130

L30 1 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 1,3-Benzodioxole-5-carboxamide, N-phenyl-4-[(phenylmethyl)seleno]- (9CI)  
 MF C21 H17 N O3 Se

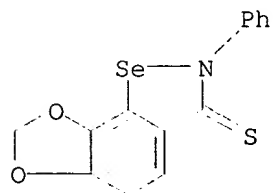


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

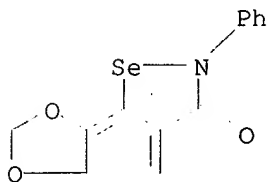
=> d scan 115

L15 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN [1,3]Dioxolo[4,5-g]-1,2-benzisoselenazole-3(2H)-thione, 2-phenyl- (9CI)  
 MF C14 H9 N O2 S Se



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

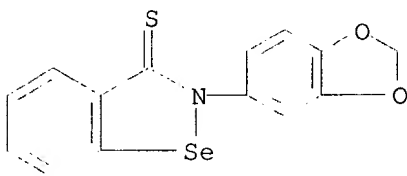
L15 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN [1,3]Dioxolo[4,5-g]-1,2-benzisoselenazol-3(2H)-one, 2-phenyl- (9CI)  
 MF C14 H9 N O3 Se



ALL ANSWERS HAVE BEEN SCANNED

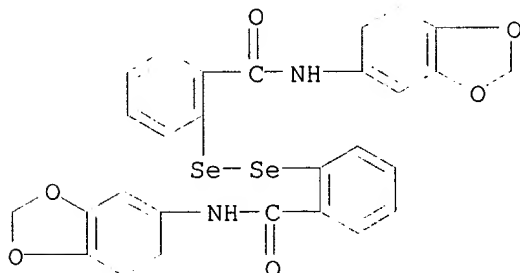
=> d sca l31

L31 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 1,2-Benzisoselenazole-3(2H)-thione, 2-(1,3-benzodioxol-5-yl)- (9CI)  
 MF C14 H9 N O2 S Se



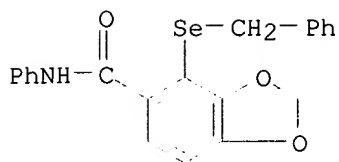
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L31 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, 2,2'-diselenobis[N-1,3-benzodioxol-5-yl]- (9CI)  
 MF C28 H20 N2 O6 Se2



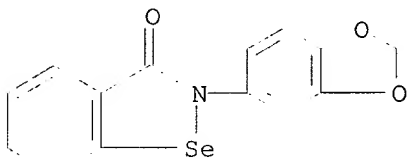
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L31 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 1,3-Benzodioxole-5-carboxamide, N-phenyl-4-[(phenylmethyl)seleno]- (9CI)  
 MF C21 H17 N O3 Se



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

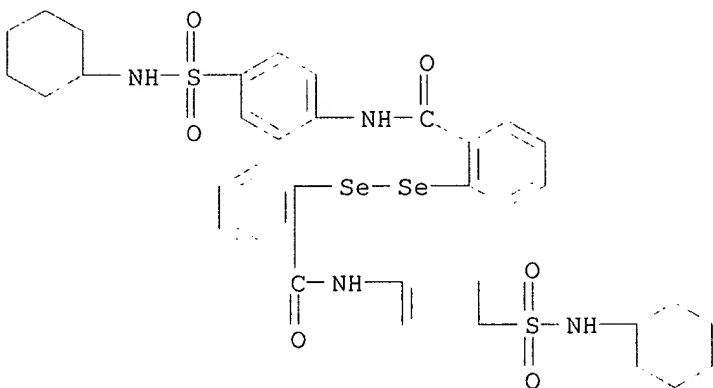
L31 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 1,2-Benzisoselenazol-3(2H)-one, 2-(1,3-benzodioxol-5-yl)- (9CI)  
 MF C14 H9 N O3 Se



ALL ANSWERS HAVE BEEN SCANNED

=> d sca 135

L35 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, 2,2'-diselenobis[N-[4-[(cyclohexylamino)sulfonyl]phenyl]- (9CI)  
 MF C38 H42 N4 O6 S2 Se2

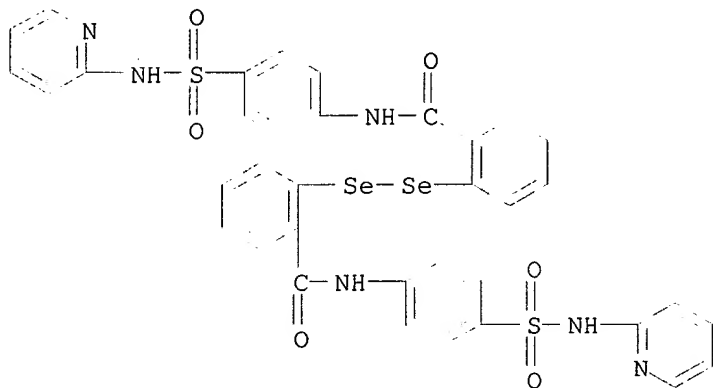


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

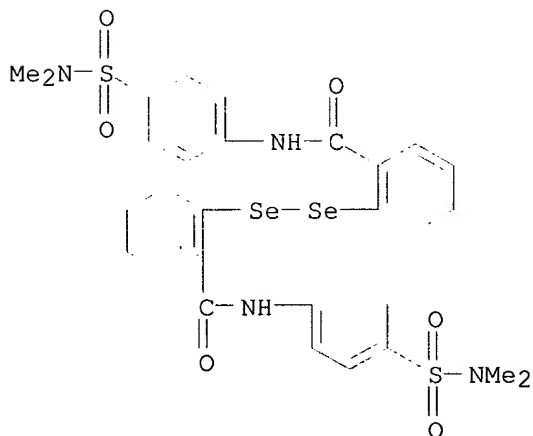


L35 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, 2,2'-diselenobis[N-[4-[(2-pyridinylamino)sulfonyl]phenyl]-  
 (9CI)  
 MF C36 H28 N6 O6 S2 Se2



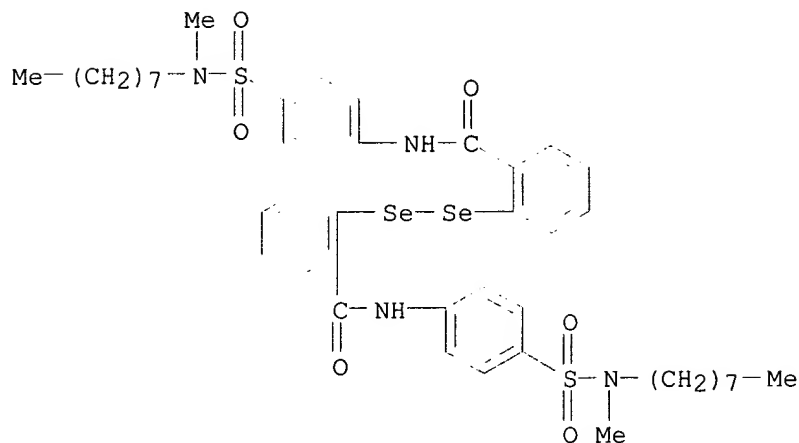
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L35 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, 2,2'-diselenobis[N-[4-[(dimethylamino)sulfonyl]phenyl]-  
 (9CI)  
 MF C30 H30 N4 O6 S2 Se2



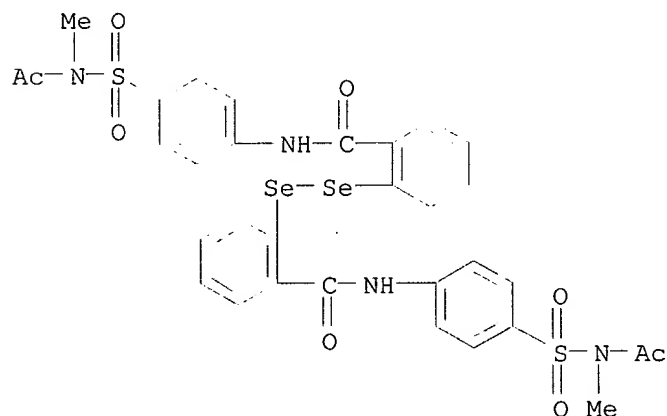
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L35 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, 2,2'-diselenobis[N-[4-[(methyloctylamino)sulfonyl]phenyl]-  
 (9CI)  
 MF C44 H58 N4 O6 S2 Se2



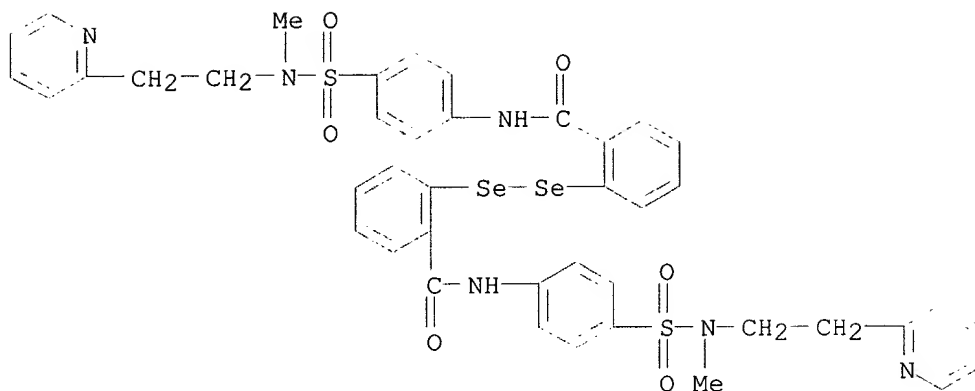
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L35 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, 2,2'-diselenobis[N-[4-[(acetylmethylamino)sulfonyl]phenyl]-  
 (9CI)  
 MF C32 H30 N4 O8 S2 Se2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L35 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, 2,2'-diselenobis[N-[4-[[methyl[2-(2-pyridinyl)ethyl]amino]sulfonyl]phenyl]- (9CI)  
 MF C42 H40 N6 O6 S2 Se2



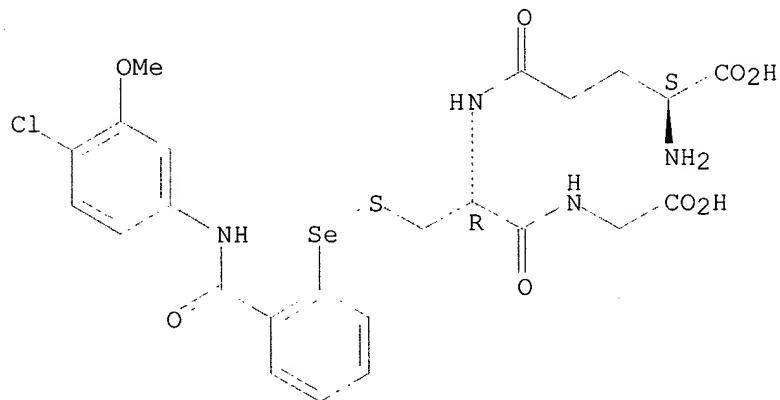
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d sca 138

L38 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Glycine, N-[S-[[2-[[ (4-chloro-3-methoxyphenyl)amino]carbonyl]phenyl]seleno]-N-L-.gamma.-glutamyl-L-cysteinyl]- (9CI)  
 MF C24 H27 Cl N4 O8 S Se

Absolute stereochemistry.

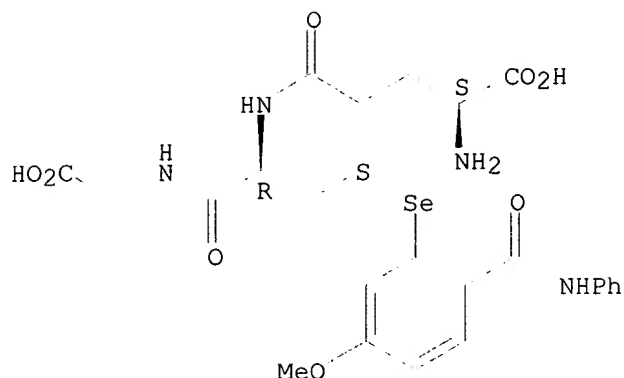


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L38 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Glycine, N-[N-L-.gamma.-glutamyl-S-[[5-methoxy-2-[(phenylamino)carbonyl]phenyl]seleno]-L-cysteinyl]- (9CI)  
 MF C24 H28 N4 O8 S Se

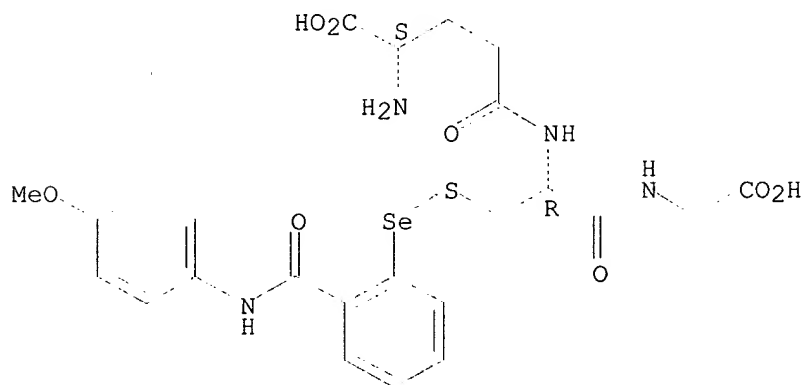
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L38 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Glycine, N-[N-L- $\gamma$ -glutamyl-S-[[2-[[4-methoxyphenyl]amino]carbonyl]phenyl]seleno]-L-cysteinyl]- (9CI)  
 MF C24 H28 N4 O8 S Se

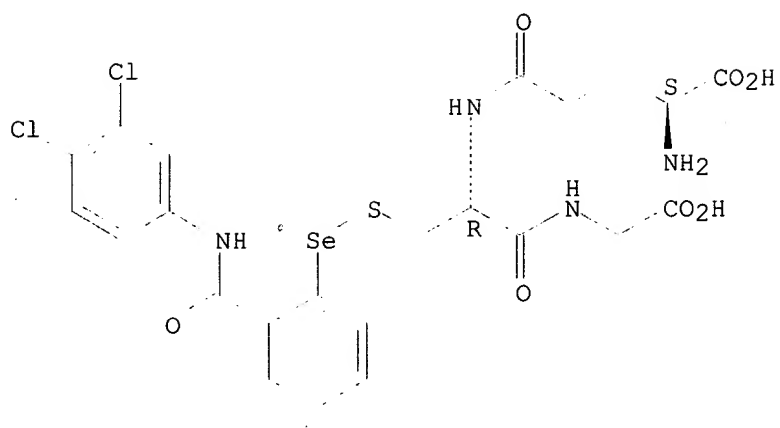
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L38 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Glycine, N-[S-[[2-[[3,4-dichlorophenyl]amino]carbonyl]phenyl]seleno]-N-L- $\gamma$ -glutamyl-L-cysteinyl]- (9CI)  
 MF C23 H24 Cl2 N4 O7 S Se

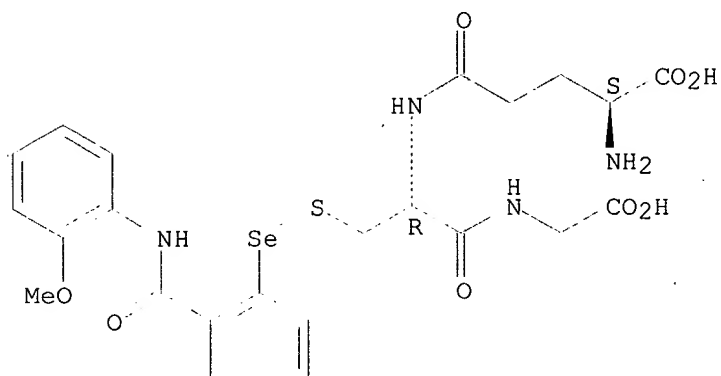
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L38 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Glycine, N-[N-L-.gamma.-glutamyl-S-[[2-[[[2-(2-methoxyphenyl)amino]carbonyl]phenyl]seleno]-L-cysteinyl]]- (9CI)  
 MF C24 H28 N4 O8 S Se

Absolute stereochemistry.



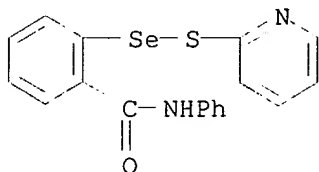
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L38 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Glycine, L-.gamma.-glutamyl-S-[[2-[(phenylamino)carbonyl]phenyl]seleno]-L-cysteinyl- (9CI)  
 MF C23 H26 N4 O7 S Se

Absolute stereochemistry.



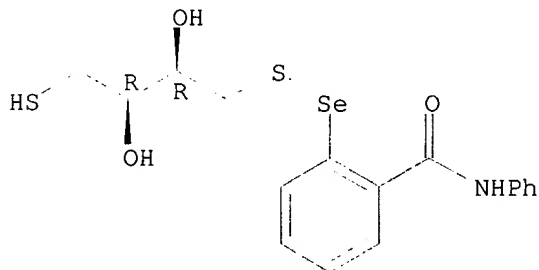
L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN 2-Pyridinesulfenoselenoic acid, 2-[(phenylamino)carbonyl]phenyl ester  
(9CI)  
MF C18 H14 N2 O S Se



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

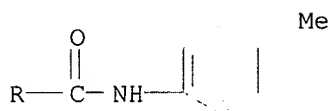
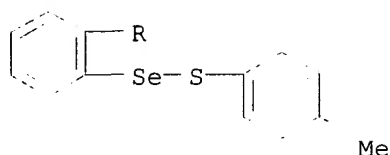
L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN 1-Butanesulfenoselenoic acid, 2,3-dihydroxy-4-mercapto-,  
2-[(phenylamino)carbonyl]phenyl ester, (R\*,R\*)- (9CI)  
MF C17 H19 N O3 S2 Se

Relative stereochemistry.



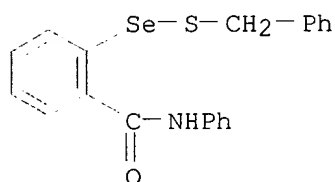
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzenesulfenoselenoic acid, 4-methyl-, 2-[[4-methylphenyl)amino]carbonyl]phenyl ester (9CI)  
MF C21 H19 N O S Se



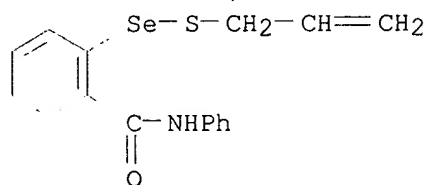
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzenemethanesulfenoselenoic acid, 2-[(phenylamino)carbonyl]phenyl ester  
 (9CI)  
 MF C20 H17 N O S Se



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

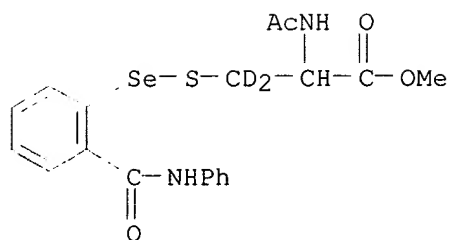
L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 2-Propene-1-sulfenoselenoic acid, 2-[(phenylamino)carbonyl]phenyl ester  
 (9CI)  
 MF C16 H15 N O S Se



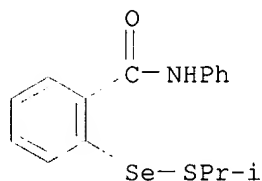
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Cysteine-3,3-d<sub>2</sub>, N-acetyl-S-[2-[(phenylamino)carbonyl]phenyl]seleno]-, methyl ester (9CI)  
 MF C19 H18 D2 N2 O4 S Se





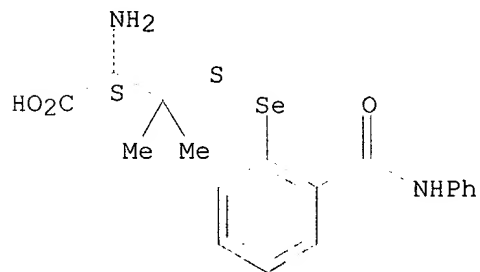
L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 2-Propanesulfenoseleonic acid, 2-[(phenylamino)carbonyl]phenyl ester (9CI)  
 MF C16 H17 N O S Se



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN D-Valine, 3-[[[2-[(phenylamino)carbonyl]phenyl]seleno]thio]- (9CI)  
 MF C18 H20 N2 O3 S Se

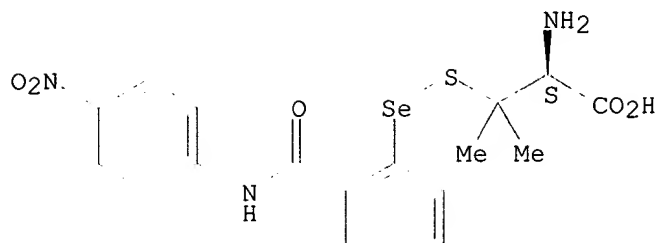
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN D-Valine, 3-[[[2-[[[4-nitrophenyl]amino]carbonyl]phenyl]seleno]thio]-  
 (9CI)  
 MF C18 H19 N3 O5 S Se

Absolute stereochemistry.

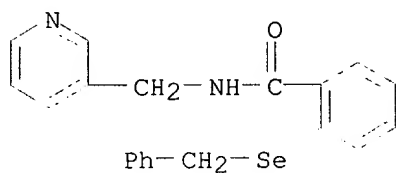


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d sca 140

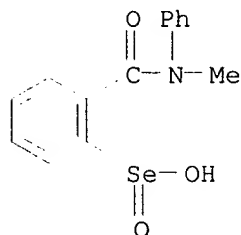
L40 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benamide, 2-[(phenylmethyl)seleno]-N-(3-pyridinylmethyl)- (9CI)  
 MF C20 H18 N2 O Se



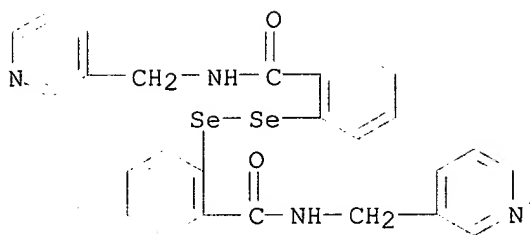
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L40 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzeneseleninic acid, 2-[(methylphenylamino)carbonyl]- (9CI)  
 MF C14 H13 N O3 Se

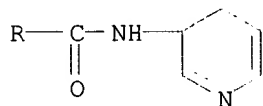
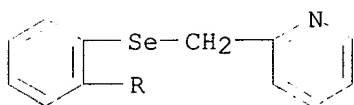


L40 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benamide, 2,2'-diselenobis[N-(3-pyridinylmethyl)- (9CI)  
 MF C26 H22 N4 O2 Se2



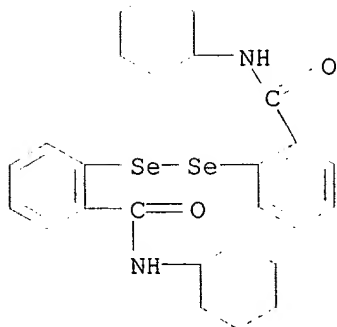
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, N-3-pyridinyl-2-[(2-pyridinylmethyl)seleno]-, monohydrochloride  
 (9CI)  
 MF C18 H15 N3 O Se . Cl H



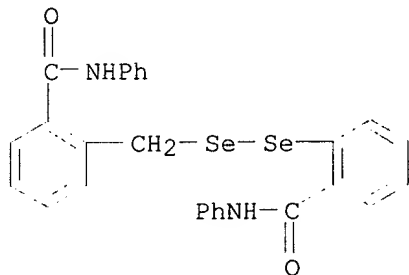
● HCl

L40 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, 2,2'-diselenobis[N-cyclohexyl]- (9CI)  
 MF C26 H32 N2 O2 Se2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, N-phenyl-2-[[[2-[(phenylamino)carbonyl]phenyl]diseleno]methyl]-  
 (9CI)  
 MF C27 H22 N2 O2 Se2

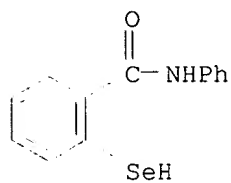


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d 151 ide can

L51 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS  
 RN 139015-80-8 REGISTRY  
 CN Benzamide, N-phenyl-2-selenyl- (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN N-Phenyl-2-carboxamidobenzeneselenol  
 MF C13 H11 N O Se  
 SR CA  
 LC STN Files: CA, CAPLUS, MEDLINE, TOXCENTER, USPAT2, USPATFULL



9 REFERENCES IN FILE CA (1962 TO DATE)  
 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 9 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 133:271642

REFERENCE 2: 132:217137

REFERENCE 3: 132:69347

REFERENCE 4: 125:230470

REFERENCE 5: 122:177623  
REFERENCE 6: 122:907  
REFERENCE 7: 118:73610  
REFERENCE 8: 118:764  
REFERENCE 9: 116:143221

=> d 152 ide can

L52 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS

RN 60940-34-3 REGISTRY

CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 2-Phenyl-1,2-benzisoselenazol-3(2H)-one

CN 2-Phenyl-1,2-benzoisoselenazol-3(2H)-one

CN Ebselen

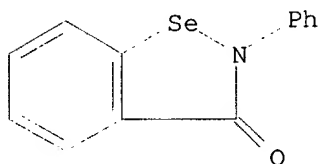
CN PZ 51

MF C13 H9 N O Se

LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, BEILSTEIN\*, BIOBUSINESS,  
BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CEN, CHEMCATS,  
CHEMINFORMRX, CIN, CSCHEM, DDFU, DRUGNL, DRUGU, DRUGUPDATES, EMBASE,  
IPA, MEDLINE, MRCK\*, PHAR, PROMT, RTECS\*, SYNTHLINE, TOXCENTER, USAN,  
USPAT2, USPATFULL

(\*File contains numerically searchable property data)

Other Sources: WHO



413 REFERENCES IN FILE CA (1962 TO DATE)

19 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

415 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 138:84749  
REFERENCE 2: 138:83310  
REFERENCE 3: 138:68712  
REFERENCE 4: 138:33174  
REFERENCE 5: 138:11174  
REFERENCE 6: 137:370035  
REFERENCE 7: 137:365444  
REFERENCE 8: 137:350476  
REFERENCE 9: 137:346030  
REFERENCE 10: 137:329273